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Interactive comment on "Biogeochemical evidence of heterotrophic N_2 fixation in the Gulf of Aqaba (Israel), Red Sea" *by* Angela M. Kuhn et al.

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Response to Comments by Reviewer 4 (Reviews are included in regular font; Responses are in bold font)

General evaluation This ms reports a 1D biogeochemical model analysis of time-series data from the Gulf od Aqaba from 2006–2014. The authors compare the behaviour of models with different diazotroph community structures representing various combinations of autotrophic and heterotrophic diazotrophs. While all model versions perform similarly with respect to surface chlorophyll, only models with diazotrophy can reproduce observed nutrient (N:P) ratios and heterotrophic diazotrophy is required to explain the vertical structure of nutrient and O2 concentrations.

In general, I find this study somewhat unconvincing. The model is overly simplistic in its mechanistic foundation and ignores processes I consider essential for this kind of analysis. While I do not dispute the potential importance of heterotrophic diazotrophy for marine biogeochemistry, the conclusions and particularly the title appear overly optimistic and not well justified. The ms also appears to have been prepared rather sloppily and not thought through. The main problem is that all diazotroph parameters are unconstrained by the data, which, as outlined below, may be a consequence of the overly simplistic nature of the model or of an inappropriate cost function. Thus, in order to turn this ms into a useful contribution, the model or the cost function (or both) must be redesigned so as to achieve sensitivity to the diazotroph-related parameters.

Response: We respond one-by-one to each of the critical points that the Reviewer raises:

With regard to the comment that "the model is overly simplistic," we would like to state that our analysis is exploratory and focused on the influence of N2 fixation, hence complexity in other parts of the ecosystem, although necessary in any global application, is intentionally minimized here. The Gulf of Aqaba is an oligotrophic system and our relatively simple model structure is able to capture the observed variability. With regard to the title being "overly optimistic and not well justified," we are happy to change the title according to this Reviewer's suggestion (also see response to detailed comment below).

With regard to the manuscript being "prepared rather sloppily and not thought through," we would like to point out that some of the information the Reviewer is requesting (i.e. literature sources of parameter values) is actually provided in the manuscript (Table 3) and discussed in the text for diazotrophic organisms (section). In our revision we will incorporate the additional information that the Reviewer is requesting, i.e. more details on the sensitivity experiments, initial conditions, more details on the ranges and literature sources for diazotrophic organisms.

With regard to "diazotroph parameters are unconstrained by the data," we would point out that this is not an issue with the model or the cost function. It is generally accepted among modellers that measured bulk properties like chlorophyll, nutrients and oxygen do not constrain most rates including rates of grazing, phytoplankton mortality and, in our case, N2 fixation (see, for example, discussion about this topic on Ward et al., 2010). No redesign of the cost function or the model will change the fact that the measured properties in the Gulf of Aqaba do not directly constrain N2 fixation rates, simply because that information is not contained in the observations. The observations capture the impact that N2 fixation only indirectly through its influence on deep-water nutrient ratios.

Ward, B.A., Friedrichs, M.A.M., Anderson, T.R., Oschlies, A., 2010. Parameter optimization techniques and the problem of underdetermination in marine biogeochemical models. J. Mar. Syst. 81, 34–43.

Specific points 1. Starting with the title, I find the wording inappropriate. While it might be possible to obtain biogeochemical evidence from a model analysis, this is certainly not the case here. I would suggest something like "Modelling heterotrophic N2 fixation ..."

Response: We will be happy to change that title as the Reviewer suggests. A tentative alternative is: "Modeling the biogeochemical effects of heterotrophic and autotrophic N2 fixation in the Gulf of Aqaba, Red Sea"

2. Model structure. Although the authors stress that they intended to analyse mechanistic assumptions (l. 15, p. 14), I find that the model is mechanistically rather weakly founded. While simplicity is of course an important goal in model development, one must take care not to over-simplify and neglect essential processes. I think this should be at least discussed thoroughly to put the results into the right perspective. The two assumptions I find most troubling are those of (1) constant (Redfield) stoichiometry of the autotrophs and (2) obligate diazotrophy, both of which are mechanistically wrong.

Fernandez-Castro et al., J. Plank. Res. 38:946 (2016), FC in the following, applied a model with variable stoichiometry and facultative diazotrophy in the subtropical North Atlantic, where the vertical distribution of N, P, and N* poses similar difficulties as in the present ms. The model of FC is otherwise very similar in structure to the present one (phytoplankton, diazotrophs, zooplankton, detritus, nutrients, DOM), so I think the differences should be discussed, particularly with respect to the relations among stoichiometry, export and remineralisation.

Response: We will be happy to further discuss the implications of our model assumptions and compare our model and results to those of Fernandez-Castro et al. in our revised manuscript. With regard to the particular assumption mentioned by the Reviewer, namely constant (Redfield) stoichiometry of the autotrophs and obligate diazotrophy, we would like to comment that the overwhelming majority of models (including those used in IPCC projections) assume constant stoichiometry and, where diazotrophy is explicitly included, obligate diazotrophy. In our revision we will include additional sensitivity experiments to show the implications of variable stoichiometry of the diazotrophs. The question of obligate diazotrophy may be boil down to semantics because autotrophic diazotrophs that aren't fixing N2 would behave like a non-diazotrophic phytoplankton, which are included in our model. We would also like to comment that our focus is not on the physiology of diazotrophs, which is analyzed in more detail by Fernandez-Castro et al. and citations therein. We acknowledge that modeling diazotrophic cells N allocation mechanisms is important to understand how they are diazotrophs are able to fixate N2 under conditions that are traditionally thought to limit the process. We will happily bring attention to this previously missing piece of information in our introduction and discussion.

Comparing the parameter settings between FC and the present model, I notice a very strong discrepancy (more than a factor of 10) in the initial-slope parameter (alpha) for photosynthesis in diazotrophs, although the units are the same in both models. It is not clear from the ms how or why the very low alpha was chosen (no reference given and not optimised). But it appears to be an important parameter given that the analysis is about the vertical structure and alpha basically defines how deep in the water column autotrophic N2 fixation can occur.

Response: Our values of alpha are within the range of values typically used in ecosystem models with similar formulations (see Doney et al. 1996; Fennel et al., 2001; Fennel et al., 2002; Schartau and Oschlies 2003; Fennel et al., 2006; Moore et al., 2004). Please also notice that while FC's our alpha parameters share the same notation, they may not refer to the same parameter because our light limitation formulations are not the same. It is not straightforward to compare these values directly to each other. We will be happy to further discuss these considerations in our revised manuscript. Nevertheless, we would also like to note that FC's alpha values were subjectively adjusted from the original model configuration by Pahlow et al., 2013. FC report these parameters were adjusted to reduce the depth of N2 fixation in their model results and even then, they obtain significant differences between the simulated and observed vertical structure of N2 fixation. To us, these differences in parameter values simply exemplify the fact that transferring parameters measured in laboratory cultures to mathematical models that represent the real ocean, and/or transporting parameters from one model to another is challenging and corresponds to a different discussion in itself.

Doney, S., D. M. Glover, R. G., Najjars, 1996. A new coupled, one-dimensional biological-physical model for the upper ocean: Applications to the JGOFS Bermuda Atlantic Time- series Study (BATS) site. Deep-Sea Research II, Vol 43, No. 2-3 pp. 591-624.

Fennel, K., M. Losch, J. Schröter and M. Wenzel, 2001. Testing a marine ecosystem model: Sensitivity analysis and parameter optimization. Journal of Marine Systems 28/1-2, p.45-63

Fennel, K., Spitz, Y.H., Letelier, R., Abbott, M.R., 2002. A deterministic model for N2 fixation at stn. ALOHA in the subtropical North Pacific Ocean. Deep-Sea Res. II 49, 149–174.

Fennel, K., Wilkin, J., Levin, J., Moisan, J., O'Reilly, J.E., Haidvogel, D., 2006. Nitrogen cycling in the Middle Atlantic Bight: Results from a three-dimensional model and implications for the North Atlantic nitrogen budget. Glob. Biogeochem. Cycles 20, 14. doi:10.1029/2005GB00245.

Schartau, M., Oschlies, A., 2003. Simultaneous data-based optimization of a 1D-ecosystem model at three locations in the North Atlantic: Part I - Method and parameter estimates. J. Mar. Res. 61, 765–793.

Moore, J.K., Doney, S., Lindsay, K., 2004. Upper ocean ecosystem dynamics and iron cycling in a global three-dimensional model. Glob. Biogeochem. Cycles 18.

Another parameter that appears rather low is the maximum growth rate of the autotrophic diazotrophs. For example, Holl Montoya, J. Phycol. 44:929 (2008) re- ported growth rates greater than 0.6/d for Trichodesmium grown in a chemostat, so a maximum (actually potential) rate parameter of 0.25/d appears unrealistically low. My impression is that these low settings reduce diazotrophy too much, maybe just compensating for the assumption of obligate diazotrophy but maybe also being responsible for the requirement of aphotic N2 fixation in the present model.

Response: Please note that the maximum growth rate in the model is temperature dependent and that 0.25/d is the reference value at 0 degrees C (as stated in Table 3). At typical water temperatures in the Gulf of Aqaba of 20 degrees C this results in an actual maximum growth rate of 0.97/d, close to the value mentioned by the Reviewer.

Further, the authors say that the diazotroph parameters were unconstrained by the data and that the parameter setting were taken from the literature, but do not provide references in Table 3 or elsewhere. The ms also does not say how it was determined that the parameters were unconstrained by the data. This seems inappropriate to me, since this is specifically a model study about diazotrophy, so I expect that great care is taken to select appropriate parameter settings. The fact that the diazotroph parameters are unconstrained by the data makes the choice of data appear questionable to me. In my view, the data should be able to constrain the most important aspects of a model's performance, and if this is not the case, one should try to either find better data or develop a better cost function (see below). The problem is that the inability to constrain the model parameters with the data implies that the associated processes are actually irrelevant. The simple fact that the authors observe better model performance when including diazotrophs implies that the associated parameters must have an effect, so I expect that a better cost function can in fact be designed which is capable of constraining those paramenters.

Response: With regard to the Reviewer's assertion that "parameter setting were taken from the literature, but do not provide references in Table 3 or elsewhere," we would like to point to Table 2 which lists ranges for each parameter from the published literature with the corresponding references (see columns 3 and 6).

In response to the comment that we do "not say how it was determined that the parameters were unconstrained by the data": Showing that measurements of chlorophyll, nutrients and oxygen do not constrain N2 fixation rates is not within the intended scope of this paper. In order to clarify, what we here mean by "unconstrained" is that, for example, chlorophyll measurements alone cannot provide any information about how much chlorophyll is due to diazotrophs and how much is due to non-diazotrophs. Therefore, this variable alone is unable to help in the determination of diazotrophic parameters (i.e., the parameters are unconstrained). The systematic calibration method we use relies on using direct observational counterparts (i.e., from the same location at least) to compare to the model output. From previous knowledge and experience using optimization

methods, we understand that we would need comprehensive N2 fixation and/or size-structured diazotrophs biomass data in order to constrain all diazotrophs parameters.

With regard to the comment that "the choice of data appear questionable to" the Reviewer, we would like to respond that we used all the data that was available. The suite of available measurements is very typical of multi-year oceanographic time series (most aren't as comprehensive and well-funded as the HOT and BATS programs).

With regard to the cost function we refer to the last paragraph in our response to the first comment.

3. Model evaluation. The authors report that they performed sensitivity analyses to obtain information of sensitive model parameters but they do not say how the sensitivity was quantified nor present any results from the sensitivity analyses. This could well be done in the supplement, but it es important for those who want to work with the model later.

Response: We will be happy to include that information in the Supplement.

The authors mention that they considered the first year of the model simulations as spinup but do not say how the model was initialised (from observations? what about the non-observed variables?). From my own experience with 1D modelling, one year is a rather short period for a spinup. Did the authors try longer spinups in order to find out whether the model is sufficiently close to a quasi-steady-state after one year? This should be discussed as well. It is this kind of omission, together with missing entries in the list of references (e.g., Fernandez 2011 and Smith 1936), that leaves an impression of sloppiness.

Response: We will be happy to include this additional information in the revised manuscript.

4. Parameter estimation. The authors apply RMSEs of absolute concentrations to obtain a measure of model-data misfit. This cost function will not be sensitive to large relative deviations if the absolute concentrations are low. Thus, it is only logical that the inability of the model to reproduce the negative N* in the surface waters "is not a source of large data-model discrepancies" (l. 8, p. 12). Introducing relative-error information or local scaling into the cost function could help here. The most important shortcoming of the authors' cost function, however, is that it neglects error correlations, see, e.g., Schartau et al., Biogeosci. 14:1647 (2017).

Response: Our cost function does indeed scale depending on the data type by weighing the contributions from the different variables by their standard deviations.

5. Figures. The use of log-scales in Fig. 9 makes it impossible to see the differences among models and between models and data. Please use a linear scale.

Response: We will be happy to provide the plots on a linear scale to illustrate why we have chosen the log-scale.

6. Conclusions. As it stands, the conclusions are not sufficiently supported be the model analysis described. In particular, the conclusions about aphotic N2 fixation are compromised by the choice of unrealistic parameter values constraining autotrophic diazotrophy to the very surface. If inferences about heterotrophic diazotrophy are to be drawn, at least the parameters determining the depth distribution of autotrophic diazotrophy must be analysed with a detailed sensitivity analysis. The current analysis cannot say whether the deep N signal is really due to aphotic N2 fixation or exported material from the surface.

Response: As per our responses above, the parameters for autotrophic diazotrophs are fully consistent with the existing literature.

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